Problems of Theoretical Interpretation of COLTRIMS Results on Ionization of Helium by Fast Bare-Ion Impact

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Abstract

In a series of recent papers, the authors argued that the experimental resolution is responsible only for a part of the marked discrepancies between theory and experiment in the COLTRIMS studies on ion-impact ionization of helium. They also pointed out that the respective theoretical treatments based on time-independent scattering theory lack account for effects of the projectile coherence, which potentially can resolve the remaining disagreement. It is shown by means of time-dependent scattering theory that the projectile-coherence effects have no impact on the cross section, in contrast to those due to the target coherence. The results and conclusions of the usual time-independent formulation remain unaltered both in the case of the first-order approximation and in the case of higher-order approximations for the on-shell T-matrix.

Keywords: *Ion-impact ionization; COLTRIMS; projectile coherence*

1 Introduction

Ionization processes in collisions of charged projectiles with atomic systems are of fundamental importance for the physics of interaction of particles and radiations with matter. The basic theory of such processes in the case of fast ionic projectiles is well established (see, for instance, the textbooks [1–4]). In particular, it is expected that at[1] $|Z_p|/v_p \ll 1$, where Z_p and v_p are the projectile charge and velocity, respectively, the perturbation theory should be well applicable. The emergence of the cold-target-recoil-ion-momentum spectroscopy (COLTRIMS) [5, 6] made it possible to measure fully differential cross sections (FDCS) for the ionizing ion-atom collisions with high precision, thus providing a new, very stringent test of the theory. In this context, a theoretical explantation of the COLTRIMS results on singly ionizing 100 Mev/u $C^{6+} + He$ ($Z_p/v_p \approx 0.10$) [7] and 1 Mev/u $H^{+} + He$ ($Z_p/v_p \approx 0.16$) [8] collisions at small momentum transfer presents a real challenge. Specifically, so far none of well-known approaches has been able to obtain a reasonable agreement with the measured electron angular distributions in a P-plane that contains the projectile momentum but is perpendicular to the scattering plane. At the same time, all approaches reasonably explain the experimental data for the scattering plane (see, for instance, Ref. [9] and references therein).

The discrepancies between theory and experiment in the 100 Mev/u $C^{6+} + He$ case [7] were attributed in Ref. [10] to experimental uncertainties of the measurements

[1] Atomic units (a.u.) in which $\hbar = e = m_e = 1$ are used throughout unless otherwise stated.

Proceedings of the International Conference 'Nuclear Theory in the Supercomputing Era — 2014' (NTSE-2014), Khabarovsk, Russia, June 23–27, 2014. Eds. A. M. Shirokov and A. I. Mazur. Pacific National University, Khabarovsk, Russia, 2016, p. 132.

http://www.ntse-2014.khb.ru/Proc/Kouzakov.pdf.

which are due to a finite energy and angle resolution, as well as to a velocity spread of the He gas atoms in a supersonic jet caused by its nonzero temperature. However, this explanation was later refuted in Ref. [11] where the experimental data of Ref. [7] were analyzed with a Monte Carlo event generator based on quantum theory. Later, in a series of papers [12–14], it was argued that the experimental resolution can explain only part (less than 50% [14]) of the discrepancies between theory and experiment in the C^{6+} problem. It was further suggested that the remaining part of the discrepancies can be attributed to the so-called projectile coherence. The first statement is relevant to the FWHM values in the discussed measurements [7]. Since this issue concerns the particular experimental method and procedures, it is beyond the scope of the theoretical analysis. Therefore, the present contribution is focused on the second statement that attributes the discrepancies to the projectile-coherence effects.

As formulated in Ref. [13], in analogy to classical optics and in accordance with Huygens' principle, the projectile transverse coherence length is given by $\Delta r \approx \lambda L/2a$, where a and L are the width of the collimating slit and its distance to the target, respectively, and λ is the de Broglie wavelength of the projectile. If the projectile coherence length is larger than the spatial extent of the target (i. e., of the He atom), the projectile is coherent and incoherent otherwise. For example, the transverse coherence length of the projectile beam in the 100 Mev/u $C^{6+} + \mathrm{He}$ experiment [7] was estimated as $\Delta r \approx 10^{-3}$ a.u. [13] thus suggesting that the C^{6+} projectiles were strongly incoherent in that experiment. This fact has a very important consequence, namely that the conventional time-independent formulation of quantum scattering theory is not applicable in the C^{6+} case. Indeed, this formulation follows from the nonstationary one, which treats time-dependent scattering of wave packets under an assumption that the colliding wave packets are sufficiently well delocalized (localized) in coordinate (momentum) space [3, 4].

In this contribution, it is analyzed and discussed, using an approach based on time-dependent quantum scattering theory, how the properties of the projectile wave packet can alter the conclusions of conventional time-independent treatments for the discussed COLTRIMS experiments. The paper is organized as follows. Section 2 delivers a general theoretical formulation in terms of projectile and target wave packets. Then, in Section 3, basic approximations for the on-shell T-matrix are presented. In Section 4, the wave-packet effects are analyzed and discussed. Finally, conclusions are drawn in Section 5.

2 General theory

Suppose the initial state of the ionic projectile in momentum space, as it is prepared in a COLTRIMS experiment, to be given by the wave packet $\Phi_p(\mathbf{q}_p)$, whereas that of the He atomic target to be given by $\Phi_T(\mathbf{q}_T)$. Then, according to the time-dependent scattering theory, the FDCS corresponding to the discussed experimental situation [7, 8] where only the momenta of ejected electron $\mathbf{k}_e$ and recoil He^+ ion $\mathbf{k}_I$ are measured while the final projectile momentum remains undetermined, is evaluated as [15]

$$d\sigma = \frac{d\mathbf{k}_e}{(2\pi)^3}\frac{d\mathbf{k}_I}{(2\pi)^3}\int\frac{d\mathbf{q}_p}{(2\pi)^3}\int\frac{d\mathbf{q}_T}{(2\pi)^3}\frac{2\pi}{v_z(\mathbf{q}_p)}\,\delta\big(E_e + I_1 - \mathbf{v}(\mathbf{q}_p)\cdot\mathbf{Q}(\mathbf{q}_T)\big) \times |\mathcal{T}_{fi}|^2|\Phi_p(\mathbf{q}_p)|^2|\Phi_T(\mathbf{q}_T)|^2, \quad (1)$$

where

$$\mathbf{Q}(\mathbf{q}_T) = \mathbf{k}_e + \mathbf{k}_I - \mathbf{q}_T$$

is the momentum-transfer function,

$$\mathbf{v}(\mathbf{q}_p) = c\,\mathbf{q}_p \Big/ \sqrt{q_p^2 + M_p^2c^2}$$

is the projectile velocity function, and $v_z(\mathbf{q})$ is its projection onto the direction of the mean projectile momentum,

$$\int \frac{d\mathbf{q}_p}{(2\pi)^3}\,\mathbf{q}_p|\Phi_p(\mathbf{q}_p)|^2 = \mathbf{k}_p. \tag{2}$$

The δ function in Eq. (1) reflects energy conservation. In its argument, kinetic energies of the target and recoil ion are neglected compared both to the electron kinetic energy E_e and to the ionization potential I_1, and the energy-transfer function $T(\mathbf{q}_p, \mathbf{q}_T)$ is approximated as follows:

$$T(\mathbf{q}_p, \mathbf{q}_T) = c\sqrt{\mathbf{q}_p^2 + M_p^2c^2} - c\sqrt{\left[\mathbf{q}_p - \mathbf{Q}(\mathbf{q}_T)\right]^2 + M_p^2c^2} \approx \mathbf{v}(\mathbf{q}_p)\cdot\mathbf{Q}(\mathbf{q}_T). \tag{3}$$

If the wave packets Φ_p and Φ_T are sufficiently well peaked about the respective mean momenta $\mathbf{k}_p$ and $\mathbf{k}_T$, the on-shell T-matrix $\mathcal{T}_{fi}$ and the functions $\mathbf{v}(\mathbf{q}_p)$ and $v_z(\mathbf{q}_p)$ in the integrand of (1) are accurately approximated by their values taken at these mean momenta. The remaining integrations over $\mathbf{q}_p$ and $\mathbf{q}_T$ then disappear as the normalization integrals for Φ_p and Φ_T [3]. As a result, the FDCS is given by [9]

$$\frac{d^3\sigma}{dE_e d\Omega_e d\Omega_p} = \frac{k_e E_p'^2}{(2\pi)^5c^4}\frac{k_p'}{k_p}\,|\mathcal{T}_{fi}|^2, \tag{4}$$

where E_p' and k_p' are the final projectile energy and momentum. It should be noted that the condition of the well localized wave packets in momentum space is usually supposed to be met in scattering experiments. If for some reason it is not the case, one should take into account the wave-packet effects in the corresponding theoretical treatment.

3 Basic approximations for T-matrix

Collisions of fast charged particles with atomic systems are usually treated to the lowest order in projectile-target interaction. The nonrelativistic lowest-order perturbation amounts to the first Born approximation (FBA) and results for the on-shell T-matrix in [1]

$$\mathcal{T}_{fi}^{\mathrm{FBA}} = \frac{4\pi Z_p}{Q^2}\,\rho_{fi}(\mathbf{Q}), \tag{5}$$

with Z_p being the projectile charge and

$$\rho_{fi}(\mathbf{Q}) = \langle\Psi_f|\sum_{j=1}^{2} e^{i\mathbf{Q}\cdot\mathbf{r}_j}|\Psi_i\rangle,$$

where $\Psi_{i(f)}$ is the ground-state (final-state) wave function of He.

Effects beyond the FBA are typically estimated within the second Born approximation (SBA). For the present case, it takes the form

$$\mathcal{T}_{fi}^{\mathrm{SBA}} = \mathcal{T}_{fi}^{\mathrm{FBA}} + \delta\mathcal{T}_{fi}^{\mathrm{SBA}}, \tag{6}$$

where the SBA contribution evaluates as [9]

$$\delta\mathcal{T}_{fi}^{\mathrm{SBA}} = \sum_n \int \frac{d^3p}{(2\pi)^3}\frac{4\pi Z_p}{(\mathbf{Q}-\mathbf{p})^2}\frac{4\pi Z_p}{p^2}\frac{\left[\rho_{fn}(\mathbf{Q}-\mathbf{p}) - 2\delta_{fn}\right]\left[\rho_{ni}(\mathbf{p}) - 2\delta_{ni}\right]}{\mathbf{v}_p\cdot\mathbf{p} + \varepsilon_i - \varepsilon_n + i0}. \tag{7}$$

Here the sum over n runs over all helium states with energies ε_n, the terms $\sim v_p p^2/k_p$ are neglected in the denominator of the Green's function in the integrand.

The projectile–target nucleus interaction plays no role in FBA which assumes a single collision between the projectile and the ejected electron and treats the initial and final projectile's states as plane waves. It can be taken into account within the distorted-wave Born approximation (DWBA) [3]. To construct the distorted waves, one can involve the straight line or eikonal approximation that proved to be very useful in treatments of near-forward scattering of particles with short de Broglie wavelength. Neglecting the change in the projectile velocity, that is, $\mathbf{v}_p = \mathbf{v}'_p$, and assuming the z axis to be directed along the incident projectile momentum, one gets [9]

$$\mathcal{T}_{fi}^{\mathrm{DWBA}} = \int d^2b \, (v_p b)^{2i\eta} \int \frac{d^2q}{(2\pi)^2} \, e^{i\mathbf{q}\cdot\mathbf{b}} \, \mathcal{T}_{fi}^{\mathrm{FBA}}(\mathbf{Q}-\mathbf{q}), \tag{8}$$

where $\mathbf{b}$ can be viewed as an impact parameter vector, Z_T is the (effective) charge of the target nucleus, $\eta = Z_p Z_T / v_p$ is the Sommerfeld parameter, and $\mathbf{q}$ is perpendicular to the z axis. The $\mathbf{b}$ integration in Eq. (8) can be carried out analytically (see Ref. [9]).

4 Results and discussion

Let us examine, using general formula (1), the role of the projectile wave packet. First, consider the FBA on-shell T-matrix (5). In this case, it is a function of the momentum transfer only, that is $\mathcal{T}_{fi} = \mathcal{T}_{fi}^{\mathrm{FBA}}\big(\mathbf{Q}(\mathbf{q}_T)\big)$, and therefore it is not involved in the integral over $\mathbf{q}_p$. Thus the $\mathbf{q}_p$ integration is governed by the properties of the projectile initial wave function $\Phi_p(\mathbf{q}_p)$ in the case of discussed experiments. According to Refs. [13, 14], the transverse coherence length in the 100 Mev/u C^{6+} + He experiment [7] was $\Delta r \approx 10^{-3}$ a.u. This value is related to the spatial extent of freely propagating projectile wave packet in real space $\Psi_p(\mathbf{r}_p, t)$ when it reaches the collision region (at the moment $t = 0$ [3]). Hence, we can estimate the transverse width of the wave packet in momentum space

$$\Phi_p(\mathbf{q}_p) = \int d\mathbf{r} \, e^{-i\mathbf{q}_p\cdot\mathbf{r}_p} \, \Psi_p(\mathbf{r}_p, t=0)$$

as[2] $\Delta p \sim 1/\Delta r \approx 10^3$ a.u. This number is very large in the atomic scale, but it appears to be insignificant as far as the projectile velocity is concerned. Indeed, the width in the velocity space is $\Delta v \simeq c\,\Delta p \Big/ \sqrt{k_p^2 + M_p^2 c^2} \sim 0.04$ a.u., thus in terms of velocity space, the wave packet $\Phi_p(\mathbf{q}_p)$ is very well peaked about the mean value of $\mathbf{v}_p = c\,\mathbf{k}_p \Big/ \sqrt{k_p^2 + M_p^2 c^2}$ ($v_p = 58.6$ a.u.). Hence the projectile velocity functions in the integrand of (1) are accurately approximated as $\mathbf{v}(\mathbf{q}_p) = \mathbf{v}_p$ and $v_z(\mathbf{q}_p) = v_p$, and the integration over $\mathbf{q}_p$ reduces to the normalization integral for Φ_p. As a result, we are left with the $\mathbf{q}_T$ integration where an absolute square of the FBA T-matrix on the energy shell is convoluted with an absolute square of the target wave packet $|\Phi_T(\mathbf{q}_T)|^2$.

In a recent theoretical analysis [9] of the 100 Mev/u C^{6+} + He experiment [7], the target wave packet was effectively taken into account by convoluting the cross section (4) with a 2D Gaussian-like momentum distribution function that also mimicked the effect of experimental uncertainties of the measurements. The latter uncertainties are due to a finite energy and angle resolution as well as to a velocity spread of the He gas atoms in the supersonic jet caused by its nonzero temperature. The results of the convolution of the FBA calculations with the 2D Gaussian-like momentum distribution function are presented in Fig. 1 in comparison with experiment. Different values of momentum-transfer uncertainties, ΔQ_x and ΔQ_y (or FWHM), are

[2]Note that the shape of a freely propagating wave packet does not vary with time in momentum space, i. e., $|\Phi_p(\mathbf{q}_p, t)|^2 = |\Phi_p(\mathbf{q}_p)|^2$.

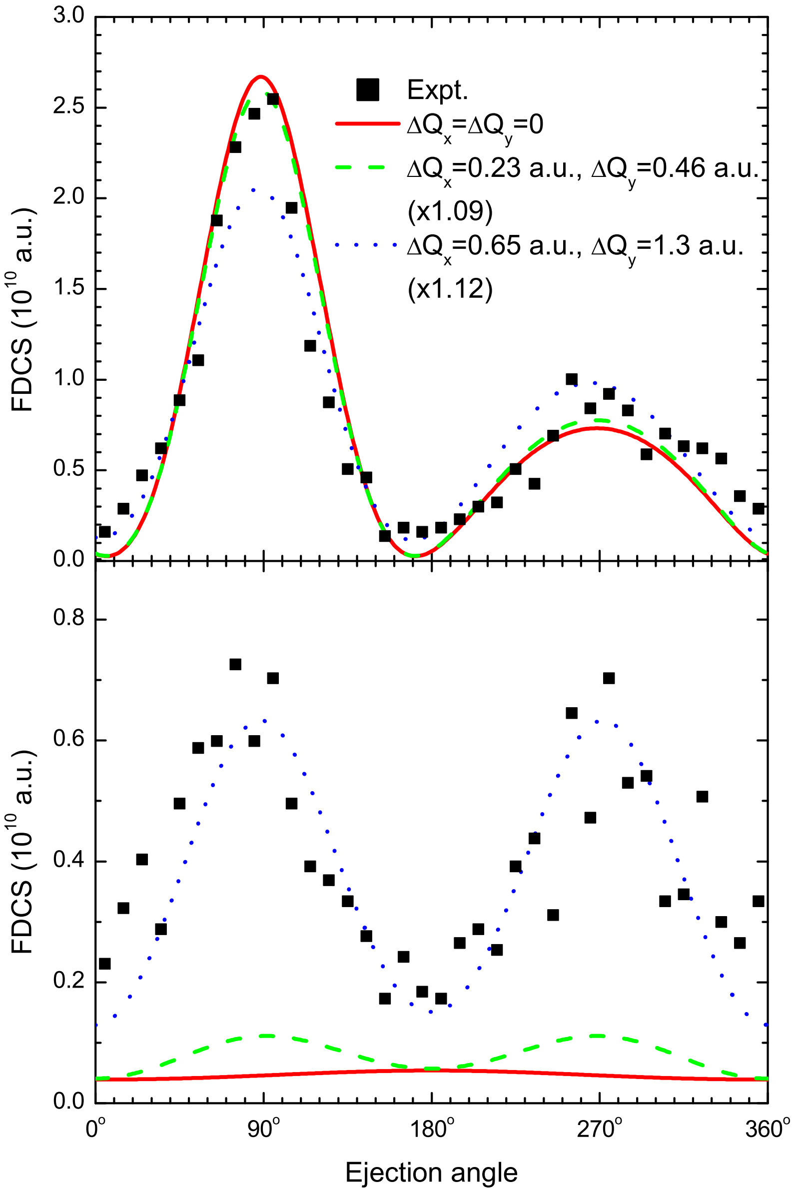

Figure 1: The FBA values for the angular distributions of the ejected electron in the scattering (top panel) and perpendicular (bottom panel) planes convoluted with experimental uncertainties. The kinetic energy of the ejected electron is $E_e = 6.5$ eV. The momentum transfer is $Q = 0.75$ a.u. All experimental and theoretical FDCS values are shown as normalized intensities relative to the FBA cross section for $Z_e = 1$. See Ref. [9] for details.

considered. The case of no uncertainties, $\Delta Q_x = \Delta Q_y = 0$, amounts to unconvoluted FBA calculations, while the FWHM values of $\Delta Q_x = 0.23$ a.u. and $\Delta Q_y = 0.46$ a.u. reported in Ref. [16] are supposed to correspond to the temperature of the He gas atoms of 1–2 K [11, 16]. It can be seen that the inclusion of uncertainties according to Ref. [16] insignificantly influences the FBA calculations in the scattering plane and only slightly reduces the large discrepancy in intensity between theory and experiment in the perpendicular plane. At the same time, it changes the theoretical angular distribution in the perpendicular plane resembling the experimental two-peak structure.

The latter observation hints at the importance of the experimental uncertainty effects in the perpendicular plane. This is illustrated in Fig. 1 by the results of convolution of the FBA calculations with the momentum uncertainties of $\Delta Q_x = 0.65$ a.u. and $\Delta Q_y = 1.3$ a.u. These values correspond to the temperature of the He gas atoms of 8–16 K which is eight times larger than that of Ref. [16]. Remarkably, the increase of temperature provides a reasonable agreement between the theory and experiment in the perpendicular plane, though it somewhat worsens the agreement in the scattering plane. This finding supports the results of Ref. [10] where continuum distorted wave calculations were convoluted with experimental uncertainties.

As remarked in Ref. [14], while it is not surprising that the convolution of FBA with the initial projectile wave packet does not change the FDCS, a proper theoretical test of a potential influence of the projectile coherence should be performed within a higher-order model. In particular, the authors of Ref. [14] suggested that a small value of Δr can lead to an incoherent contribution to the FDCS from the FBA and higher-order amplitudes (particularly, those containing projectile-nucleus interaction [16]). Higher order collision mechanisms, including those due to projectile-nucleus interaction, enter the SBA (6) and DWBA (8) models. Using them in the general formula (1), we find that in both cases the on-shell T-matrix depends not only on the momentum-transfer function $\mathbf{Q}(\mathbf{q}_T)$, as in the FBA case, but also on the projectile momentum variable $\mathbf{q}_p$. However, the latter dependence enters only through the projectile velocity function $\mathbf{v}(\mathbf{q}_p)$,

$$\mathcal{T}_{fi} = \mathcal{T}_{fi}^{\mathrm{SBA/DWBA}}\big(\mathbf{Q}(\mathbf{q}_T), \mathbf{v}(\mathbf{q}_p)\big). \tag{9}$$

As in the FBA case discussed above, we make use of the fact that the projectile wave packet Φ_p is very well peaked in velocity space, setting $\mathbf{v}(\mathbf{q}_p) = \mathbf{v}_p$ and $v_z(\mathbf{q}_p) = v_p$ in the integrand and performing the remaining integration over $\mathbf{q}_p$ as the normalization integral for Φ_p. Thus the effect of the projectile wave packet disappears, and we are left again with the convolution of FDCS with $|\Phi_T(\mathbf{q}_T)|^2$.

5 Summary and conclusions

In conclusion, using a rigorous approach based on time-dependent scattering theory, we find no evidence that the projectile wave packet (or the projectile coherence) can play any appreciable role. Moreover, both in the case of the first-order model (FBA) and in the case of higher-order models (SBA and DWBA), only the target wave packet appears to be important. This result is mainly due to the fact that, in the discussed experiments, only the momenta of final target fragments (the ejected electron and the recoil He^+ ion) were measured, whereas the final projectile momentum remained undetermined. One can readily see that determining the momentum transfer directly, that is, by measuring the final projectile momentum $\mathbf{k}'_p$ instead of the He^+ momentum $\mathbf{k}_I$, would bring about a huge effect of the initial projectile wave packet $\Phi_p(\mathbf{q}_p)$. Indeed, in such a case, the on-shell T-matrix $\mathcal{T}_{fi}$ varies strongly as a function of the momentum transfer $\mathbf{Q}(\mathbf{q}_p) = \mathbf{k}'_p - \mathbf{q}_p$ in the region of localization of $\Phi_p(\mathbf{q}_p)$, and hence the above cancelation of the projectile wave packet is not possible. This observation directly reflects the smallness of the coherence length of the projectile beam in comparison with the spatial extent of the target since the T-matrix is closely related to the Fourier transform of the target potential [3]. It thus shows that in the situation of the discussed experiments, one should compare the spatial extent of the target (the atomic size) with the coherence length of the target beam rather than the projectile beam.

Acknowledgments

This work was supported by the Russian Foundation for Basic Research (Grant No 14-01-00420-a).

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